Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\formIIexact.str

```
chain nodes :
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39
40 41 42 43
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27
chain bonds :
1-7 3-39 5-8 8-9 8-10 10-11 10-15 13-18 17-19 19-20 19-21 21-22 21-25
23-28 27-29 29-30 29-31 31-32 31-33 33-34 34-36 36-37 36-38 39-40 39-41 41-42
41-43
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25
25-26 26-27
exact/norm bonds :
1-2 1-5 3-39 8-9 8-10 10-15 13-14 13-17 19-20 19-21 21-25 23-24 23-27
29-30 29-31 31-33 36-37 36-38 39-41 41-42
exact bonds :
1-7 2-3 3-4 4-5 5-8 10-11 13-18 14-15 15-16 16-17 17-19 21-22 23-28
24-25 25-26 26-27 27-29 31-32 33-34 34-36 39-40 41-43
isolated ring systems :
containing 1 : 13 : 23 :
```

G1:H,CH3

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 33:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\AAAformIIexact.str

chain nodes : 7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 ring nodes : 1 2 3 4 5 13 14 15 16 17 23 24 25 26 27 chain bonds : 1-7 2-44 3-39 4-45 5-8 8-9 8-10 10-11 10-15 13-18 14-47 16-46 17-19 19-20 19-21 21-22 21-25 23-28 24-49 26-48 27-29 29-30 29-31 31-32 31-33 33-34 33-50 33-51 34-36 34-52 34-53 36-37 36-38 39-40 39-41 41-42 41-43 ring bonds : 1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25 25-26 26-27 exact/norm bonds : 1-2 1-5 3-39 8-9 8-10 10-15 13-14 13-17 19-20 19-21 21-25 23-24 23-27 29-30 29-31 31-33 36-37 36-38 39-41 41-42 exact bonds : 1-7 2-3 2-44 3-4 4-5 4-45 5-8 10-11 13-18 14-15 14-47 15-16 16-17 16-46 17-19 21-22 23-28 24-25 24-49 25-26 26-27 26-48 27-29 31-32 33-34 33-50 33-51 34-36 34-52 34-53 39-40 41-43 isolated ring systems : containing 1 : 13 : 23 :

G1:H,CH3

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 3.3:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 34:CLASS 36:CLASS 37:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS L4 STRUCTURE UPLOADED

='> d

L4 HAS NO ANSWERS

L4

STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14 ful

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\AAAAAAAAAAXcorrect.str

```
chain nodes :
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39
40 41 42 43 44 50 51 52 53 54 56 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27 45 46 47
                                                                 48
                                                                   49
59 60 61
chain bonds :
1-7 2-76 3-39 4-75 5-8 8-9 8-10 10-11 10-15 13-18 14-74 16-73 17-19
19-20 19-21 21-22 21-25 23-28 24-72 26-71 27-42 29-31 29-30 29-61 31-32 31-33
33-34 33-65
                          36-37 36-38 39-40
                                                                    44-47 44-54 45-50
33-66 34-36 34-63 34-64
                                               39-41
                                                      42-43
                                                             42-44
46-69
48-70 49-51 51-52 51-53 53-56 53-59 57-62 58-68 60-67
ring bonds :
1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17 \quad 23-24 \quad 23-27 \quad 24-25
25-26 26-27 45-46 45-49 46-47 47-48 48-49 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-7 8-9 8-10 10-11 10-15 13-18 19-20 19-21 21-22 21-25 23-28 29-31 29-30
31-32 31-33 36-37 36-38 39-40 39-41 42-43 42-44 44-47 44-54 45-46 45-49 45-50
46-47
47-48 48-49 51-52 51-53 53-56 53-59 57-58 57-61 57-62 58-59 59-60 60-61
exact bonds :
1-2 \quad 1-5 \quad 2-3 \quad 2-76 \quad 3-4 \quad 3-39 \quad 4-5 \quad 4-75 \quad 5-8 \quad 13-14 \quad 13-17 \quad 14-15 \quad 14-74 \quad 15-16
16-17 16-73 17-19 23-24 23-27 24-25 24-72 25-26 26-27 26-71 27-42 29-61 33-34
33-65
33-66 34-36 34-63 34-64 46-69 48-70 49-51 58-68 60-67
isolated ring systems :
```

10519889 - Compound Search

containing 1 : 13 : 23 :

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS

22:CLASS

23:Atom 24:Atom 25:Atom 26:Atom, 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS

34:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

44:CLASS

45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:CLASS 51:CLASS 52:CLASS 53:CLASS

54:CLASS

56:CLASS 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:CLASS 63:CLASS 64:CLASS

65:CLASS

66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS

2 ANSWERS

75:CLASS

76:CLASS

L1 STRUCTURE UPLOADED

=> s l1 ful

FULL SEARCH INITIATED 12:05:35 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 22 TO ITERATE

100.0% PROCESSED 22 ITERATIONS

SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\formulaII.str

```
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39
40 .41 42 43
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27
chain bonds :
1-7 3-39 5-8 8-9 8-10 10-11 10-15 13-18 17-19 19-20 19-21 21-22 21-25
23-28 27-29 29-30 29-31 31-32 31-33 33-34 34-36 36-37 36-38 39-40 39-41 41-42
41-43
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25
25-26 26-27
exact/norm bonds :
1-2 1-5 1-7 3-39 8-9 8-10 10-11 10-15 13-14 13-17 13-18 19-20 19-21
21-22 21-25 23-24 23-27 23-28 29-30 29-31 31-32 31-33 36-37 36-38 39-41 41-42
exact bonds :
2-3 3-4 4-5 5-8 14-15 15-16 16-17 17-19 24-25 25-26 26-27 27-29 33-34
34-36 39-40 41-43
isolated ring systems :
containing 1 : 13 : 23 :
```

G1:H,CH3

```
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 33:CLASS 33:CLASS 39:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS
```

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

I.1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 11:53:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1326 TO ITERATE

100.0% PROCESSED 1326 ITERATIONS

53 ANSWERS

SEARCH TIME: 00.00.01

L2 53 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 172.10 172.31

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=> s 12

L3 586 L2

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\CH3II.str

```
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39
40 41 42 43
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27
chain bonds :
1-7 3-39 5-8 8-9 8-10 10-11 10-15 13-18 17-19 19-20 19-21 21-22 21-25
23-28 27-29 29-30 29-31 31-32 31-33 33-34 34-36 36-37 36-38 39-40 39-41 41-42
41-43
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25
25-26 26-2.7
exact/norm bonds :
1-2 1-5 3-39 8-9 8-10 10-11 10-15 13-14 13-17 19-20 19-21 21-22 21-25
23-24 23-27 29-30 29-31 31-32 31-33 36-37 36-38 39-41 41-42
exact bonds :
1-7 2-3 3-4 4-5 5-8 13-18 14-15 15-16 16-17 17-19 23-28 24-25 25-26
26-27 27-29 33-34 34-36 39-40 41-43
isolated ring systems :
```

G1:H,CH3

containing 1 : 13 : 23 :

chain nodes :

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

L4 STRUCTURE UPLOADED

=> S

ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end SEARCH ENDED BY USER

=> s 14 full

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 11:54:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1278 TO ITERATE

100.0% PROCESSED 1278 ITERATIONS

45 ANSWERS

SEARCH TIME: 00.00.01

L5 45 SEA SSS FUL L4

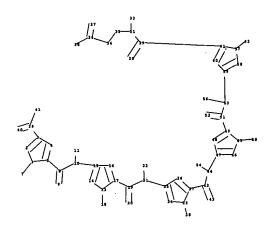
L6 585 L5

=> s 13 not 15

585 L5

L7 . 1 L3 NOT L5

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\Xcorrect.str



```
chain nodes :
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39
40 41 42 43 44 50 51 52 53 54 56 62
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27 45 46 47 48 49 57 58
59 60 61
chain bonds :
1-7 3-39 5-8 8-9 8-10 10-11 10-15 13-18 17-19 19-20 19-21 21-22 21-25
23-28 27-42 29-31 29-30 29-61 31-32 31-33 33-34 34-36 36-37 36-38 39-40 39-41
42-43
42-44 44-47 44-54 45-50 49-51 51-52 51-53 53-56 53-59 57-62
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25
25-26 26-27 45-46 45-49 46-47 47-48 48-49 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-7 8-9 8-10 10-11 10-15 13-18 19-20 19-21 21-22 21-25 23-28 29-31 29-30
31-32 31-33 36-37 36-38 39-40 39-41 42-43 42-44 44-47 44-54 45-46 45-49 45-50
46-47
47-48 48-49 51-52 51-53 53-56 53-59 57-58 57-61 57-62 58-59 59-60 60-61
exact bonds :
1-2 1-5 2-3 3-4 3-39 4-5 5-8 13-14 13-17 14-15 15-16 16-17 17-19 23-24 23-27 24-25 25-26 26-27 27-42 29-61 33-34 34-36 49-51
isolated ring systems :
containing 1 : 13 : 23 :
```

10519889 - Compound Search

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS

22:CLASS

23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS 33:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

44:CLASS

45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:CLASS 51:CLASS 52:CLASS 53:CLASS

54:CLASS

56:CLASS 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:CLASS

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l10 ful

FULL SEARCH INITIATED 11:55:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 22 TO ITERATE

100.0% PROCESSED 22 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

2 SEA SSS FUL L10 L11

Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\n=1.str

```
chain nodes :
6 8 9 10 11 12 19 20 21 22 23 29 30 31 32 33 34 35 36
ring nodes :
1 2 3 4 5 14 15 16 17 18 24 25 26 27 28
chain bonds :
1-8 3-6 5-9 9-10 9-11 11-12 11-16 14-19 18-20 20-21 20-22 22-23 22-26
24-29 28-30 30-31 30-32 32-33 32-34 34-35 35-36
ring bonds :
1-2 1-5 2-3 3-4 4-5 14-15 14-18 15-16 16-17 17-18 24-25 24-28 25-26
26-27 27-28
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 3-6 4-5 9-10 9-11 11-12 11-16 14-15 14-18 14-19
15-16 16-17 17-18 20-21 20-22 22-23 22-26 24-25 24-28 24-29 25-26 26-27 27-28
30-31
30-32 32-33 32-34 35-36
exact bonds :
5-9 18-20 28-30 34-35
```

G1:H,CH3

```
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 33:CLASS 33:CLASS 36:CLASS 36:C
```

L1 STRUCTURE UPLOADED

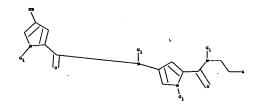
=> d L1 HAS NO ANSWERS L1 STR *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

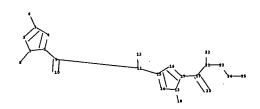
Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful FULL SEARCH INITIATED 15:34:47 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 12914 TO ITERATE

100.0% PROCESSED 12914 ITERATIONS 5471 ANSWERS SEARCH TIME: 00.00.01

L2 5471 SEA SSS FUL L1
Uploading C:\Program Files\Stnexp\Queries\10 series\10519889\n=0.str





chain nodes :
6 8 9 10 11 12 18 19 20 21 22 23 24 25
ring nodes :
1 2 3 4 5 13 14 15 16 17
chain bonds :
1-8 3-6 5-9 9-10 9-11 11-15 11-12 13-18 17-19 19-20 19-21 21-22 21-23
23-24 24-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 3-6 4-5 9-10 9-11 11-15 11-12 13-14 13-17 13-18
14-15 15-16 16-17 19-20 19-21 21-22 21-23 24-25
exact bonds :
5-9 17-19 23-24

10519889 - Compound Search '

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS

21:CLASS

22:CLASS 23:CLASS 24:CLASS 25:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14 ful

FULL SEARCH INITIATED 15:35:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 16772 TO ITERATE

100.0% PROCESSED 16772 ITERATIONS

8292 ANSWERS

SEARCH TIME: 00.00.01

L5 8292 SEA SSS FUL L4

```
chain nodes :
7 8 9 10 11 18 19 20 21 22 28 29 30 31 32 33 34 36 37 38 39 40 41
42 43
ring nodes :
1 2 3 4 5 13 14 15 16 17 23 24 25 26 27
chain bonds :
1-7 3-39 5-8 8-9 8-10 10-11 10-15 13-18 17-19 19-20 19-21 21-22 21-25 23-28
27-29 29-30 29-31 31-32 31-33 33-34 34-36 36-37 36-38 39-40 39-41 41-42 41-43
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17 23-24 23-27 24-25 25-26
26-27
exact/norm bonds :
1-2 1-5 1-7 3-39 8-9 8-10 10-11 10-15 13-14 13-17 13-18 19-20 19-21 21-22
21-25 23-24 23-27 23-28 29-30 29-31 31-32 31-33 36-37 36-38 39-41 41-42
exact bonds :
2-3 3-4 4-5 5-8 14-15 15-16 16-17 17-19 24-25 25-26 26-27 27-29 33-34 34-36
39-40 41-43
isolated ring systems :
containing 1 : 13 : 23 :
```

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

STRUCTURE UPLOADED L1

=> s l1 ful

FULL SEARCH INITIATED 11:49:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1330 TO ITERATE

100.0% PROCESSED 1330 ITERATIONS 53 ANSWERS

SEARCH TIME: 00.00.01

L2 53 SEA SSS FUL L1

=> s 12 and liposome

3 LIPOSOME

L3 0 L2 AND LIPOSOME

=> s 12 and micelle

1 MICELLE

L4 0 L2 AND MICELLE

=> s 12 and nanoparticle

0 NANOPARTICLE

L5 0 L2 AND NANOPARTICLE

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 193.81 194.02

FULL ESTIMATED COST

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=> s 12

L6 586 L2

L7 3 L6 AND LIPOSOME

=> s 16 and micelle

44319 MICELLE

L8 1 L6 AND MICELLE

=> s 16 and phospholipid 85377 PHOSPHOLIPID L9 1 L6 AND PHOSPHOLIPID

=> d ibib hitstr l6 1-3